STM induced hydrogen desorption is a method for making patterns with atomic precision on the Si (001):H and Ge(001):H surfaces. This technique can open pathways for surface electronic devices controlled with atomic precision. The dangling bond defects on the surface can be used as templates for further processing steps, e.g., attaching molecules to form a molecular wire. Still, it would be desirable to largely avoid these extra steps and use exclusively the dangling bonds for fabricating flat nanometer scale devices. However, the 1D structures formed by dangling bonds are prone to suffer from instabilities that open a band gap in the wires.

We have theoretically investigated dangling bond structures on Si(001):H and Ge(001):H with the aim of finding a ballistically conducting wire without a band-gap. Different levels of doping have been explored to see if the Fermi level can be manipulated without fundamentally changing the electronic structure of the wires, thus allowing to move the Fermi level away from the gap. Our conclusion is that such an approach is possible for Ge, while for Si the wire electrons have a strong tendency localize and open new band gaps.

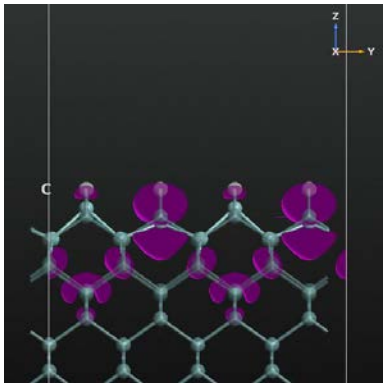

Figure: Isosurface of the DOS of the 1D band formed in the band gap of the Ge(001):H surface when a line of hydrogen atoms are removed

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On-surface chemistry: cyclodehydrogenation of PAH catalyzed by metal surfaces.

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One of the main goals in nanotechnology is to assemble low dimensional molecular networks in order to create new nano-objects. For that purpose, on-surface chemistry is one of the most powerful and suitable bottom-up approaches that can be employed. Dehydrogenation reactions of polycyclic aromatic hydrocarbons (PAH) catalyzed by metal surfaces allow a control at the atomic level of the resultant outcome, with the correct choice of the geometry of the precursor and on the type of metallic surface[1].

In this work, we show that the strength of the PAH-substrate interaction rules the competitive reaction pathways (cyclodehydrogenation versus dehydrogenative polymerisation). Starting from the same molecular precursor ($C_{57}H_{33}N_3$ or $C_{40}H_{24}N_2$ (DiPy[5]DBH) and controlling its diffusion by the nature of the supporting surface (Au(111) or Pt(111)), temperature-triggered dehydrogenation takes place to provide molecular or polymeric structures of variable dimensionality[2-3].

Combining advanced in-situ surface techniques as STM and NEXAFS with theoretical ab-initio calculations we have been able to achieve a complete understanding of the self-assembling of molecular precursors on surfaces. By merging information from these techniques and different single-crystal metal substrates, we report on the diffusion control of competitive intramolecular and intermolecular dehydrogenative processes respectively called cyclodehydrogenation and dehydrogenative polymerisation, which operate in the on-surface synthesis of N-doped fullerene, nanographene, polyaromatic network, membrane or grapheme (Fig. 1). By choosing the appropriate N-heteroaromatic precursors and by controlling their diffusion, the on-surface (cyclo)dehydrogenation can either lead to monomolecular triazafullerenes and diazahexabenzocoronenes (N-doped nanographene), or to N-doped polymeric networks.

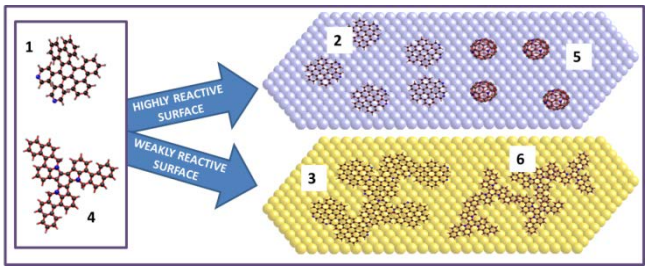

Fig. 1: The heteroaromatic precursors 1 and 4 subjected to controlled on-surface dehydrogenation. 1 and 4 may form respectively (i) N-doped triazafullerene 2 or 2,5-diazahexabenzocoronene 5 (through intramolecular cyclodehydrogenation) or (ii) branched 2D polyaromatic architectures 3 or 6 (both through intermolecular dehydrogenative polymerisation and intramolecular cyclodehydrogenation).

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Substrate-Induced Stabilization And Reconstruction Of Zigzag Edges In Graphene Nanoislands On Ni(111)

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